lsopropylpropyzamide 80045-52-9 | DTXSID40230046

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I١	/Ioaei	Performance	

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 113 °C

Global applicability domain: Inside

Local applicability domain index: 4.95e-01

Confidence level: 5.45e-01

Nearest Neighbors from the Training Set

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Hexanamide, N-phenyl- (9CI)

Measured: 95.0 Predicted: 109

Image not found

N-(2,4-

Dimethylphenyl)acetamide

Measured: 129 Predicted: 128

Image not found

Butanamide, N-phenyl-

Measured: 97.0 Predicted: 122

Image not found

Acetamide, N-(2,6-dimethylphenyl)-Measured: 183
Predicted: 138

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N-Benzylacetamide Measured: 61.0 Predicted: 79.7